AN ANALYSIS OF THE TORSION-ROTATION-VIBRATION ROTATIONAL SPECTRUM OF THE LOWEST IN-PLANE BEND AND FIRST EXCITED TORSIONAL STATE OF THE C_{1V} INTERNAL ROTOR C₂H₅CN

J. C. PEARSON, HERBERT M. PICKETT

Jet Propulsion Laboratory, California Institute of Technology, Mail Stop 183-301, 4800 Oak Grove Dr., Pasadena, CA 91109-8099

K. V. L. N. SASTRY

Department of Physics, University of New Brunswick, Fredericton, New Brunswick, E3B 5A3 Canada

C₂H₅CN (Propionitrile or ethyl cyanide) is a well known interstellar species abundantly observed in hot cores during the onset of star formation. The onset of star formation generally results in elevated temperature, which thermally populates may low lying vibrational states such as the 206 cm⁻¹ in-plane bend and the 212 cm⁻¹ first excited torsional state in C₂H₅CN. Unfortunately, these two states are strongly coupled through a complex series of torsion-vibration-rotation interactions, which dominate the spectrum. In order to understand the details of these interactions and develop models capable of predicting unmeasured transitions for astronomical observations in C₂H₅CN and similar molecules, several thousand rotational transitions in the lowest excited in-plane bend and first excited torsional state have been recorded, assigned and analyzed. The analysis reveals very strong a- and b-type Coriolis interactions and a number of other smaller interactions and has a number of important implications for other C_{3V} torsion-rotation-vibration systems. The relative importance and the physical origins of the coupling among the rotational, vibrational and torsional motions will be presented along with a full spectroscopic analysis and supporting astronomical observations.